THEOCHEM, VOLUME 59 (1989)

(*Journal of Molecular Structure, Vol. 188*)

AUTHOR INDEX

Allinger, N.L., 149
Andre, J.-M., 229
Aoki, Y., 321

Bakhshi, A.K., 205
Barbier, C., 299
Bencivenni, L., 105
Biczó, G., 429
Biondi, F., 199
Brédas, J.L., 393
Brendsdal, E., 55

Calais, J.-L., 213
Cheam, T.C., 15
Chen, B.-H., 167
Cometta-Morini, C., 79
Cyvin, S.J., 55

Danovich, D., 159
Delhalle, J., 213, 299
Devia, A., 141
Domnina, E., 159

Estrada, M., 141
Ewbank, J.D., 111

Förner, W., 231
Fukutome, H., 337

Garcia-Cuesta, I., 1
Godzik, A., 231
Goldstein, E., 149
Gribov, L.A., 175

Ha, T.-K., 79
Hofmann, D., 231

Imamura, A., 321

Jankowski, K., 67
Ji, Q.-E., 167
Jiao, K.-F., 167
Jinfeng, C., 45

Krimm, S., 15

La Manna, G., 199
Ladik, J., 205, 231, 289
Landry, D., 67
Lavrinenko-Ometsinskaya, Y.D., 193
Liegener, C.-M., 205

March, N.H., 261
Martino, F., 231
Merchan, M., 1
Minkin, V.I., 129
Miralles-Sabater, J., 1
Mosquera, R.A., 95

Nebot-Gil, I., 1
Nemzoff. G., 141
Nikitin, O.Yu., 175
Novosadov, B.K., 175

Oth, J.F.M., 79
Otto, P., 205, 277

Pichko, V.A., 129

Raitblat, L.I., 175
Ramondo, F., 105
Ríos, M.A., 95
Rossi, V., 105

Schäfer, L., 111
Seel, M., 231, 381
Shichiri, T., 313
Siam, K., 111
Simkin, B.Ya., 129
Soler, F., 67
Song, H.-Q., 167
Stafström, S., 393
Strelko, V.V., 193

Tanaka, K., 313
Topsom, R.D., 45

Van Alsenoy, C., 95
Vazquez, S., 95

Watanabe, E., 321

Yamabe, T., 313

Zakrzewski, V., 159
Zamarbide de Sosa, G., 141

THEOCHEM, VOLUME 59 (1989)

(Journal of Molecular Structure, Vol. 188)

SUBJECT INDEX

Acetic acids
Effect of hydration on the acidities of substituted acetic acids, 45

Alanine dipeptide
Ab initio force fields of alanine dipeptide in C_5 and C_7 conformations, 15

Allyl radicals
Ab initio study of the vibrational spectra of the allyl and the cyclopropyl radicals, 79

AM1 approximation
Ionization energies of azines from Green's function method in semiempirical AM1 approximation, 159

Anticholinesterase activity
Studies on the relationship between the MO indices and anticholinesterase activity of suberogorgin, 167

Aperiodic polypeptides
Effects of correlation and hydration on the electronic stucture of aperiodic polypeptides, 205

Asymmetric reaction paths
Asymmetric reaction paths for ground- and excited-state 1,3,5-hexatriene to 1,3-cyclohexadiene cyclizations, 129

Azines
Ionization energies of azines from Green's function method in semiempirical AM1 approximation, 159

Band structure
An energy-decomposition technique for the analysis of band structure and its application to polyphosphazene and its halogenated derivatives, 321

Benzenediamine, 4-(2-thiazolylazo)
Theoretical studies on the molecular structure of 1,3-benzenediamine, 4-(2-thiazolylazo), 141

C_5 conformations
Ab initio force fields of alanine dipeptide in C_5 and C_7 conformations, 15

C_7 conformations
Ab initio force fields of alanine dipeptide in C_5 and C_7 conformations, 15

Carbon sorbents
A quantum chemical study of the effect of nitrogen heteroatoms on the chemical parameters of carbon sorbents, 193

Clover-leaf like structures
Computer-assisted clover-leaf like structures of t-RNA, 67

Conformational analysis
Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level, 95

Correlation
Effects of correlation and hydration on the electronic structure of aperiodic polypeptides, 205

Cu^+/H_2O
A MO–CI study of the Cu/H_2O and Cu^+/H_2O systems, 1

Cu/H_2O
A MO–CI study of the Cu/H_2O and Cu^+/H_2O systems, 1

Cyclizations
Asymmetric reaction paths for ground- and excited-state 1,3,5-hexatriene to 1,3-cyclohexadiene cyclizations, 129

Cyclohexadiene
Asymmetric reaction paths for ground- and excited-state 1,3,5-hexatriene to 1,3-cyclohexadiene cyclizations, 129

Cyclopropyl radicals
Ab initio study of the vibrational spectra of the allyl and the cyclopropyl radicals, 79

Doping
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393

Electronic structure
Effects of correlation and hydration on the electronic structure of aperiodic polypeptides, 205
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393
The electronic structure and magnetic properties of poly (*m*-phenylcarbene), 313
End states
Green's function calculation of local perturbations and end states in polymers, 381
Exchange singularities
Exchange singularities in the RHF energy-band spectrum of metallic polymers, 213

Footballene
Kekulé structures of footballene, 55
Force fields
Ab initio force fields of alanine dipeptide in C_5 and C_7 conformations, 15

Geometry functions
Ab initio studies of structural features not eaily amenable to experiment. Part 66. Quantitative predictions of some structure–conformation relations in branched hydrocarbons from component standard geometry functions, 111
Green's function
Green's function calculation of local perturbations and end states in polymers, 381
Ionization energies of azines from Green's function method in semiempirical AM1 approximation, 159

Heteroatoms
A quantum chemical study of the effect of nitrogen heteroatoms on the chemical parameters of carbon sorbents, 193
Hexatriene
Asymmetric reaction paths for ground- and excited-state 1,3,5-hexatriene to 1,3-cyclohexadiene cyclizations, 129
Hydration
Effect of hydration on the acidities of substituted acetic acids, 45
Effects of correlation and hydration on the electronic structure of aperiodic polypeptides, 205
Hydrocarbons
Ab initio studies of structural features not eaily amenable to experiment. Part 66. Quantitative predictions of some structure–conformation relations in branched hydrocarbons from component standard geometry functions, 111
Hydroxydiazines
Ab initio study of the tautomeric equilibria of hydroxydiazines in the vapour phase. Part 3. 5-Hydroxypyrimidine and hydroxypyrazine, 199
Hydroxypyrazine
Ab initio study of the tautomeric equilibria of hydroxydiazines in the vapour phase. Part 3. 5-Hydroxypyrimidine and hydroxypyrazine, 199
Hydroxypyrimidine
Ab initio study of the tautomeric equilibria of hydroxydiazines in the vapour phase. Part 3. 5-Hydroxypyrimidine and hydroxypyrazine, 199

Ionization energies
Ionization energies of azines from Green's function method in semiempirical AM1 approximation, 159

Kekulé structures
Kekulé structures of footballene, 55

Lead dihalides
Molecular structure and vibrational frequencies of lead and tin dihalides: a SCF study, 105

Magnetic field
The effect of magnetic field on the band structure of polymers. Part 1. Static magnetic field, 289
Magnetic properties
The electronic structure and magnetic

properties of poly (*m*-phenylcarbene), 313
Many-body effects
Many-body effects in polymers: especially polyacetylene, 261
Metallic polymers
Exchange singularities in the RHF energy-band spectrum of metallic polymers, 213
2-Methoxyethanol
Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level, 95
MO indices
Studies on the relationship between the MO indices and anticholinesterase activity of suberogorgin, 167
MO–CI study
A MO–CI study of the Cu/H_2O and Cu^+/H_2O systems, 1
Molecular geometry
Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level, 95
Molecular mechanics calculations
Molecular mechanics calculations (MM2) on aliphatic nitriles, 149

Nitriles
Molecular mechanics calculations (MM2) on aliphatic nitriles, 149
Nitrogen
A quantum chemical study of the effect of nitrogen heteroatoms on the chemical parameters of carbon sorbents, 193

Oligodinucleotides
Investigation of the stability of oligonucleotides and oligodinucleotides, 277
Oligonucleotides
Investigation of the stability of oligonucleotides and oligodinucleotides, 277

Perturbation theory
An improved perturbation theory and its application to the spectral theory of polyatomic molecules, 175
Perturbations
Green's function calculation of local perturbations and end states in polymers, 381
Polarizability
Ab initio calculations of the static electric polarizability of infinite polymer chains, 299
Polyacetylene
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393
Many-body effects in polymers: especially polyacetylene, 261
PPP–UHF model of polyacetylene, 337
trans-Polyacetylene
Solitondynamicsinalternating*trans*-polyacetylene and in stacked systems, 231
Polyatomic molecules
An improved perturbation theory and its application to the spectral theory of polyatomic molecules, 175
Polyemeraldine
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393
Polymer chains
Ab initio calculations of the static electric polarizability of infinite polymer chains, 299
Polymers
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393
Exchange singularities in the RHF energy-band spectrum of metallic polymers, 213
Green's function calculation of local perturbations and end states in polymers, 381
Many-body effects in polymers: especially polyacetylene, 261
The effect of magnetic field on the band structure of polymers. Part 1. Static magnetic field, 289
Polypeptides
Effects of correlation and hydration on the electronic structure of aperiodic polypeptides, 205
Poly(*m*-phenylcarbene)
The electronic structure and magnetic properties of poly(*m*-phenylcarbene), 313

Polyphosphazene
An energy decomposition technique for the analysis of band structure and its application to polyphosphazene and its halogenated derivatives, 321
Polythiophene
Electronic structure of highly conducting conjugated polymers: evolution upon doping of polyacetylene, polythiophene, and polyemeraldine, 393
PPP-UHF model
PPP-UHF model of polyacetylene, 337

RHF energy-band spectrum
Exchange singularities in the RHF energy-band spectrum of metallic polymers, 213
t-RNA
Computer-assisted clover-leaf like structures of t-RNA, 67

SCF-LCAO-BCO method
On the self-consistent-field linear combination of atomic orbitals for bounded crystal orbitals (SCF-LCAO-BCO) method, 429
Soliton dynamics
Soliton dynamics in alternating *trans*-polyacetylene and in stacked systems, 231
Sorbents
A quantum chemical study of the effect of nitrogen heteroatoms on the chemical parameters of carbon sorbents, 193
Spectral theory
An improved perturbation theory and its application to the spectral theory of polyatomic molecules, 175
Suberogorgin
Studies on the relationship between the MO indices and anticholinesterase activity of suberogorgin, 167

Tautomeric equilibria
Ab initio study of the tautomeric equilibria of hydroxydiazines in the vapour phase. Part 3. 5-Hydroxypyrimidine and hydroxypyrazine, 199
Tin dihalides
Molecular structure and vibrational frequencies of lead and tin dihalides: a SCF study, 105

Vibrational spectra
Ab initio study of the vibrational spectra of the allyl and the cyclopropyl radicals, 79